Manufactured Solutions for Verifying CFD Boundary Conditions

A Case Study

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
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Verification

- **Code verification deals with identifying:**
  - **Coding mistakes that cause the governing equations to be solved incorrectly, or**
  - **Shortcomings of formulations or algorithms that result in undesirable or unexpected behavior.**
- **Code verification involves comparing code numerical solutions with exact solutions.**
- **Solution verification deals with quantifying numerical errors in a given solution.**
- *Code verification is especially needed when a code is believed to be free of coding and algorithmic mistakes!*

Code Verification

- In code verification, an important thing to verify is order-of-accuracy of discretization:
  - what is the observed order-of-accuracy of the numerical solution?
  - is the observed order greater than zero? (convergence)
  - Does the observed order match one's expectations?
  - If known, does the observed order match the formal accuracy of the algorithm?
- Order verification requires:
  - Mesh refinement/coarsening
  - Exact solutions to governing equations

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Methods for Obtaining Exact Solutions

Method of Exact Solutions (MES): solutions to simplified forms of governing equations

- Physically reasonable solutions, however
  - Need a new exact solution every time the boundary conditions are changed
  - An exact solution may not exist for a given equation set.
  - Exact solutions which do exist may lack generality and therefore even multiple exact solution test suites may fail to test all code capabilities
  - Exact solutions which do exist can be difficult to evaluate accurately (*e.g.,* series or integral solutions)
  - Sometimes can only be found on unbounded domains
  - Often contain singularities which make it difficult to determine order of accuracy

Method of Manufactured Solutions (MMS): solutions to general form of governing equations or 'modified' general form

- Are exact solutions, too!
  - Often can use same mfg solution with different sets of boundary conditions
  - Can, in principle, test full set of code capabilities (greater coverage)
  - Easy to evaluate
  - Can avoid singular and discontinuous solutions
  - May require the addition of a non-physical source term to the governing equations
  - Analytic computation of source term is usually complex

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The Method of Manufactured Solutions

1. Create (*i.e.,* manufacture) a solution that satisfies the governing equations (with possibly the addition of a source term) on the domain of interest.
2. Operate on this manufactured solution with the differential operator for the interior equations to determine the source term which balances the equations
3. If no source exists in the governing equations (as in Euler and Navier-Stokes), then the code must be modified to include a source term.
4. Provide the source term input to the code,
5. Compute any fluxes or other needed to balance the boundary conditions using the mfg soln. (e.g., flux BC's)
6. Proceed with order verification.

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Example

1) Consider Laplace's Equation on Ω :

$$\nabla^2 u = 0.$$

2) Manufacture a solution u^*.

3) Operate (analytically) on u^* with ∇^2 :

$$\nabla^2 u^* = f^*.$$

4) Provide the source term f^* to the code.

5) Operate (analytically) on u on $\partial\Omega$ with boundary operators :

$\partial u^* / \partial n = g^*$

6) Run the code with the additional source term to obtain numerical solutions on a series of systematically refined grids.

7) Compare the numerical solutions with u^* to determine the spatial order of accuracy for the code.

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Boundary Condition Issues

- For Dirichlet & Neumann boundary conditions, one can often construct the manufactured solution independently of the specific conditions to satisfied by u^* on the boundary.
- For certain boundary conditions (a.k.a. hardwired boundary conditions), one often manufactures the solution so u^* directly satisfies the boundary conditions.
- For hyperbolic and parabolic equation sets, only constraints corresponding to incoming characteristics need to be satisfied.

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Boundary Conditions Tested by MMS

Boundary Condition	Equation Set
slip	Euler
no-slip, adiabatic	Navier-Stokes, RANS
no-slip, isothermal	Navier-Stokes, RANS
subsonic outflow	Euler
supersonic outflow	Euler

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Surface Definition

Define a function $\mathcal{F} = \mathcal{F}(x, y, z)$ such that $\mathcal{F} = C$ defines a surface for any constant C.

The normal is defined by $\hat{n} = \dfrac{\nabla \mathcal{F}}{\|\nabla \mathcal{F}\|}$.

The manufactured solution can be constructed so that any variable ϕ satisfies a Dirichlet (ϕ constrained) or Neumann ($\dfrac{\partial \phi}{\partial n}$ constrained) condition on $\mathcal{F} = C$.

Solid Surface Velocity Conditions

A) Slip condition:

$$\vec{F}\cdot\hat{n}=\begin{bmatrix}0\\ p\hat{n}\\ 0\end{bmatrix}\Leftrightarrow v_n=0$$

$$\Rightarrow \nabla\mathcal{F}\cdot\vec{v}=0\Leftrightarrow \mathcal{F}_x u+\mathcal{F}_y v+\mathcal{F}_z w=0 \text{ on the surface } \mathcal{F}=C_{\mathrm{s}}$$

Can be different surfaces in the same solution.

B) No-slip condition:

$$\vec{v}=0\Leftrightarrow u=v=w=0 \text{ on the surface } \mathcal{F}=C_{\text{n-s}}$$

The manufactured solution is defined everywhere in space. The choice of domain determines which conditions can be tested.

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Solid Surface Thermal Conditions

Adiabatic boundary :

$$\frac{\partial T}{\partial n} = 0 \Leftrightarrow \nabla T \cdot \hat{n} = 0$$

$$\Rightarrow \mathcal{F}_x T_x + \mathcal{F}_y T_y + \mathcal{F}_z T_z = 0 \text{ on } \mathcal{F} = C_{\text{n-s}}$$

Can be the same surface.

Isothermal boundary :

$$T = T_c \text{ on } \mathcal{F} = C_{\text{n-s}}$$

Note: a thermal condition is always required with the no-slip BC. The Navier-Stokes equations are under-constrained without one.

Outflow Conditions

Subsonic outflow :

$v_n > 0, \quad M_n < 1, \quad p = p_c$ **along a portion of the surface** $\mathcal{G} = C_o$

same surface

Supersonic outflow :

$v_n > 0, \quad M_n > 1$ **along a portion of the surface** $\mathcal{G} = C_o$

To close the problem we create a constant pressure surface with variable normal Mach number.

Using these boundary conditions, not enough degrees of freedom remain to test inflow conditions with the same solution.

The Surfaces

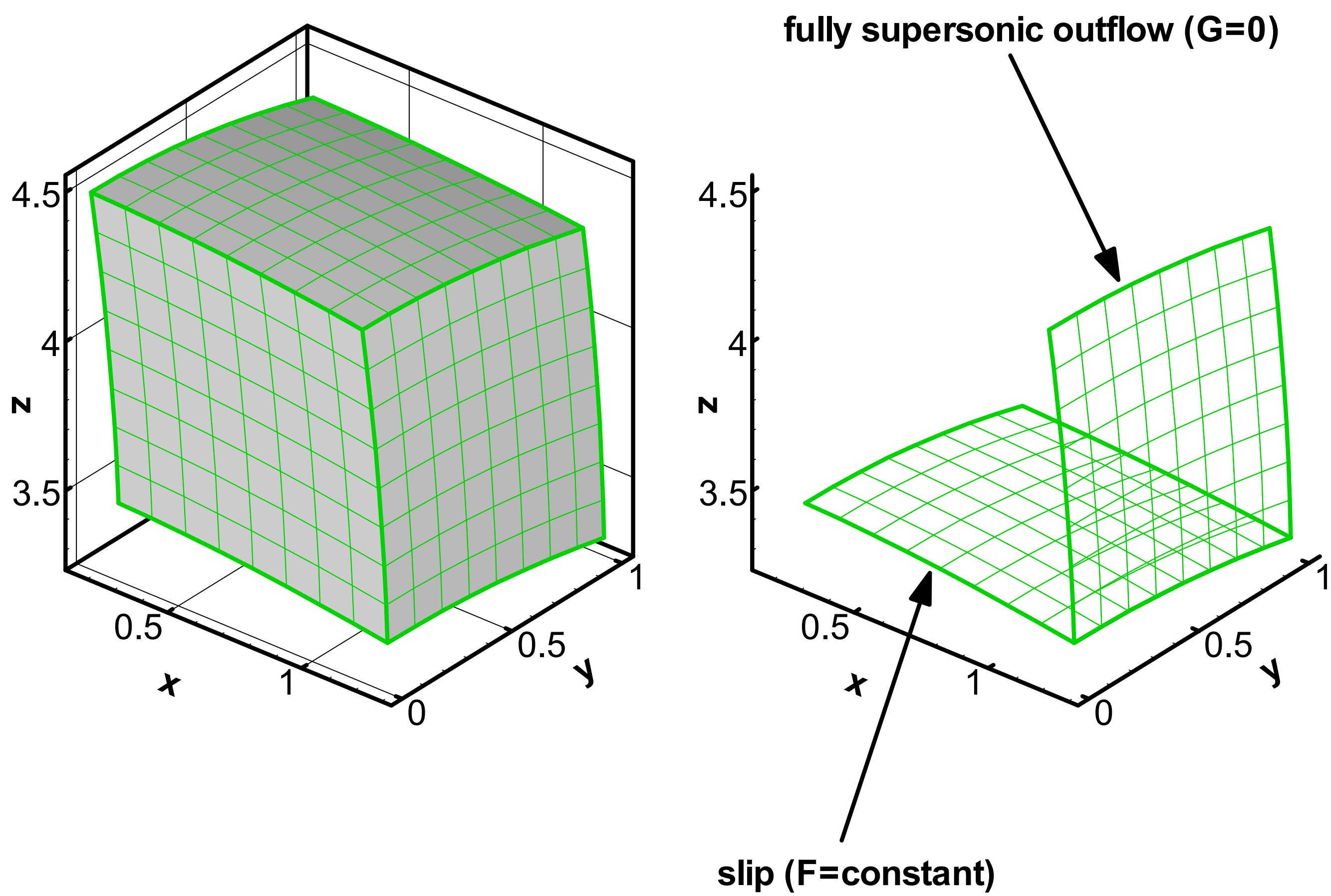
$\mathcal{F} = \frac{1}{2}\cos(A_f x)\cos(B_f y) - z$ **Test solid surface BCs on $\mathcal{F} = C$.**

$\mathcal{G} = x - \frac{1}{2}\cos(A_g y)\sin(B_g z) - \frac{\pi}{4}$ **Test outflow BCs on $\mathcal{G} = C$.**

$\mathcal{H} = -y$ **No BCs tested on $\mathcal{H} = C \Rightarrow$ simplicity okay.**

A six-sided domain can be constructed which is bounded by $\mathcal{F}_{\min} < \mathcal{F} < \mathcal{F}_{\max}$, $\mathcal{G}_{\min} < \mathcal{G} < \mathcal{G}_{\max}$, $\mathcal{H}_{\min} < \mathcal{H} < \mathcal{H}_{\max}$.

Computational Domain 1



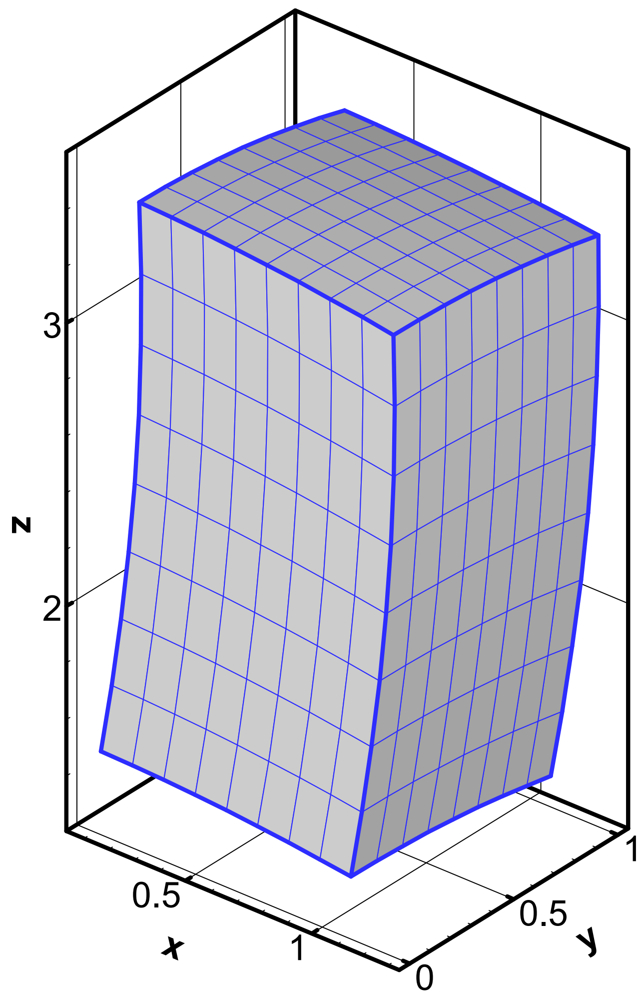
Tests Using Domain 1

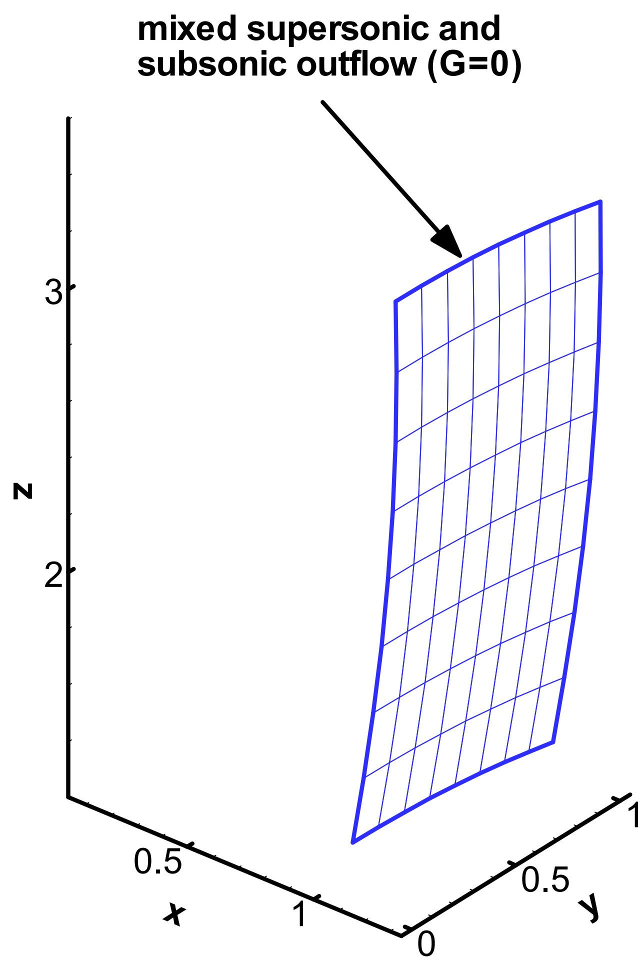
1. All-Dirichlet, Green-Gauss gradient reconstruction
2. All-Dirichlet, Equally-Weighted Least-Squares
3. All-Dirichlet, Inverse-Distance-Weighted Least Squares
4. Outflow on G=0, Dirichlet elsewhere, Green-Gauss
5. Slip on F=C, Dirichlet elsewhere, Green-Gauss

Euler equations for all these tests.

Note that the mesh is (non-orthogonal) structured and is derived from an analytic map to facilitate mesh refinement.

Computational Domain 2



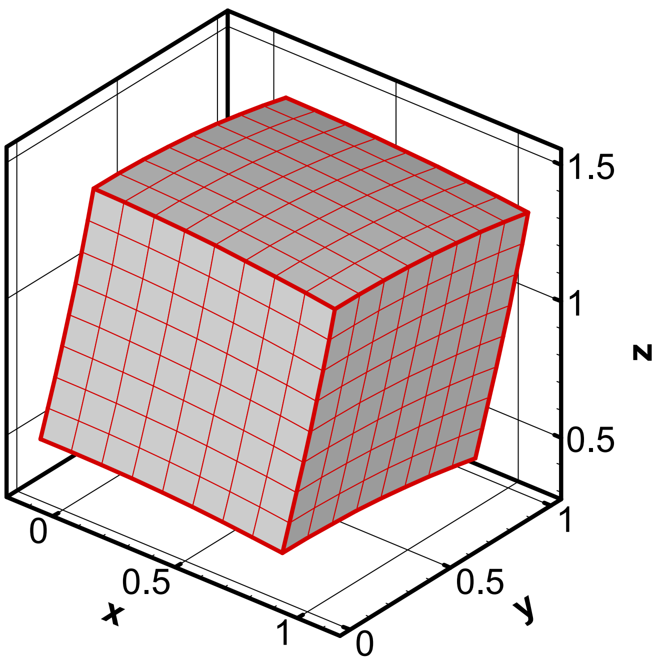


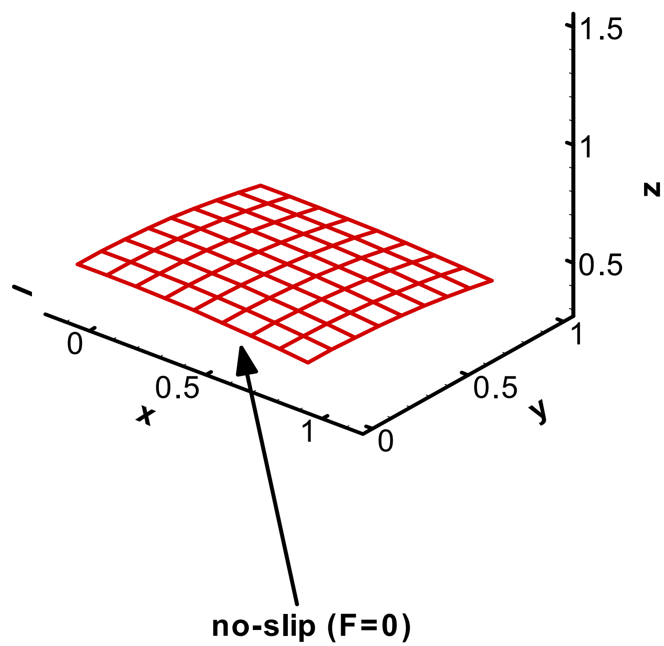
Tests Using Domain 2

6. Mixed subsonic and supersonic outflow on G=0, Dirichlet elsewhere, Green-Gauss

Euler equations solved.

Computational Domain 3





Tests Using Domain 3

7. Dirichlet everywhere, Green-Gauss
8. No-slip with Adiabatic, Dirichlet elsewhere, Green-Gauss
9. No-slip with Isothermal, Dirichlet elsewhere, Green-Gauss

Navier-Stokes equations solved.

The Manufactured Solution

- The manufactured solution is defined in terms of *p*, *u*, *v*, *w*, *T*.
- These variables are defined primarily using products of sinusoidal functions for smoothness and differentiability.
- The manufactured solutions for these variables conform to the previously mentioned constraints for testing BC's.
- See AIAA2005-0088 for the derivation, statement, and in-depth discussion of the manufactured solution.

Premo

premo (Latin) – to squeeze (compress)

Develop simulation capabilities to perform compressible flow calculations.

- Compressible subsonic through hypersonic
- Laminar through turbulent regimes
- Inviscid and viscous flows
- Steady state and transient
- Chemically reacting flow
- Multi-physics coupling
- Verified capabilities
- Arbitrary body motion
- Finite Volume, Unstructured Mesh
- Adaptivity

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Test 1

Test Setup:

- Solving Euler Equations
- Dirichlet boundary conditions applied to all dependent variables
- Green-Gauss gradient reconstruction

First-try Results: observed 2nd-order of accuracy in density, pressure, and velocity

Conclusions:

- Because observed order matched expected order, there is strong evidence that the interior (Euler) equations are correctly solved.
- Green-Gauss order was verified as well.
- MMS testing is facilitated by first testing the interior equations before applying complex boundary conditions.
- Because the Dirichlet conditions, as implemented in Premo, are infinite order of accuracy, the interior equations are best tested using Dirichlet conditions.

Test 2

Test Setup:

- Solving Euler Equations
- Dirichlet boundary conditions applied to all dependent variables
- Equally-weighted Least-squares gradient reconstruction

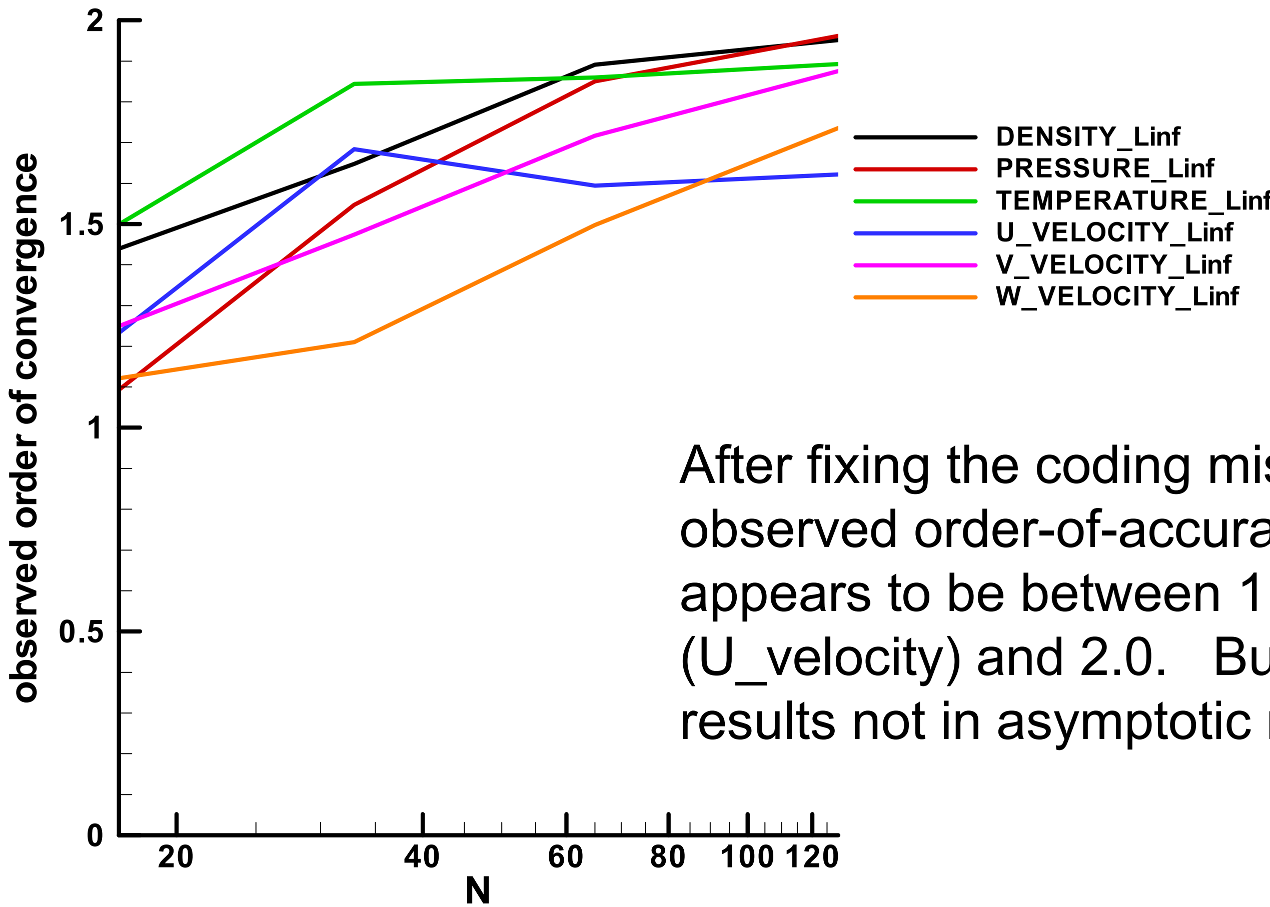
Results on First Try: Observed order of accuracy was between 0.5 and 1.0 for all variables (see AIAA2004-2629).

Explanation:

- First tried to justify the observed order by citing papers in the literature which showed similar behavior, saying this must be the formal order.
- Then, through an independent effort, discovered a coding mistake within an index swapping algorithm for the directional derivative in the gradient calculation.

Corrected the coding mistake and re-tested (see next slide)

Equally-Weighted Least Squares



After fixing the coding mistake, observed order-of-accuracy appears to be between 1.5 (U_velocity) and 2.0. But results not in asymptotic regime.

Manufactured Solution Modified

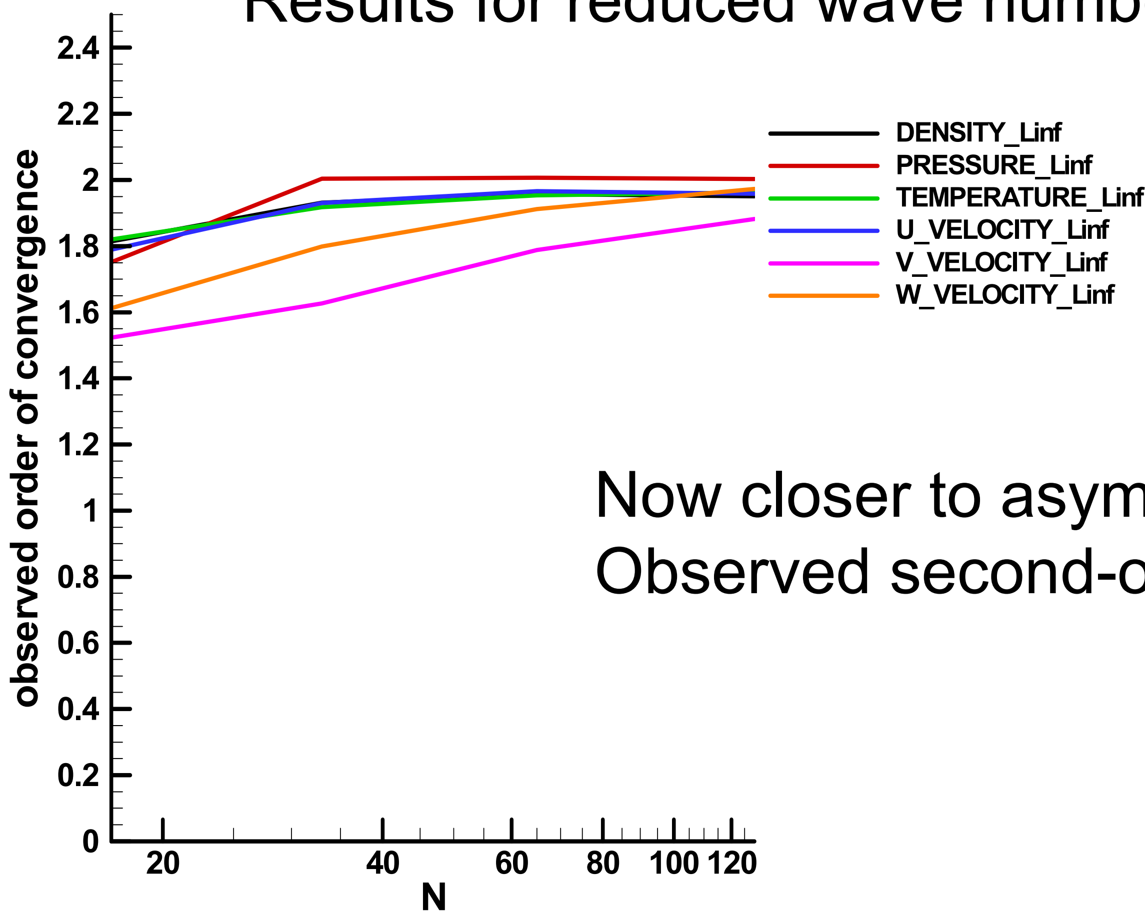
Modifications made to attain asymptotic regime with previous meshes.

Approach:

- Decrease wave number parameters in sinusoidal functions used to define *F* and *G.*
- Decrease wave numbers and constants used to define the solution variables *p*, *u*, *v*, *w*, *T*.

Equally-weighted Least Squares

Results for reduced wave numbers



Now closer to asymptotic regime.
Observed second-order

Test 2 - Conclusions

Conclusions:

- When formal order-of-accuracy is unknown, don't be too quick to blame the numerical algorithm if observed order is lower than expected,
- MMS can indicate that a coding mistake probably exists, but will not automatically find it for you,
- Even after a coding mistake has been found, results may still not match the expected order-of-accuracy because other problems remain,
- Attaining the asymptotic regime on practical mesh sizes depends heavily on one's choice of parameters in the manufactured solution. Need parameter values that result in a problem that is not too hard, but not too easy. Start with values which result in an easy problem because requires less computer time,
- MMS results provides strong evidence that equally-weighted gradient reconstruction option is now working correctly,

Test 3

Test Setup:

- Solving Euler Equations
- Dirichlet boundary conditions applied to all dependent variables
- Inverse-Distance Least-squares gradient reconstruction

Results: see next slide

Conclusions:

- Seems to be approaching second-order but not quite in asymptotic regime on U_velocity.

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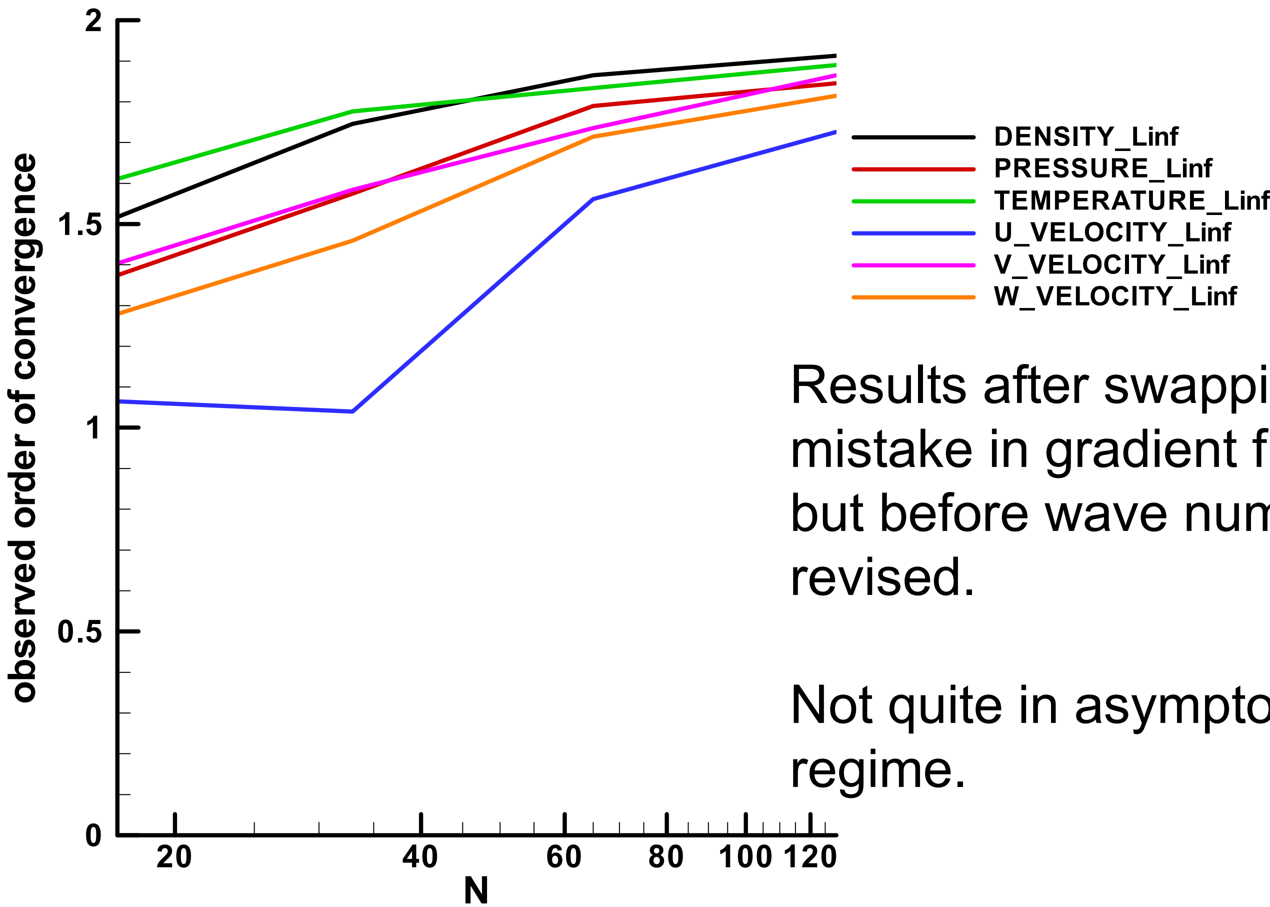
Inverse-Distance-Weighted Least Squares



Results after swapping mistake in gradient fixed, but before wave numbers revised.

Not quite in asymptotic regime.

Test 4

Test Setup:

- Solving Euler Equations
- Supersonic Outflow Boundary condition on G=0
- Dirichlet boundary conditions applied to all dependent variables elsewhere
- Green-Gauss gradient reconstruction

Results: observed 2^{nd}-order of accuracy in density, pressure, and velocity (see AIAA2004-2629)

Conclusions:

- Because observed order matched expected order, there is strong evidence that the Outflow boundary condition is correctly solved.

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Test 5

Test Setup:

- Solving Euler Equations,
- Slip boundary condition on F=C,
- Dirichlet conditions applied elsewhere,
- Green-Gauss gradient reconstruction

Results on First Try:

- Negative order-of-accuracy observed in all variables!

Explanation:

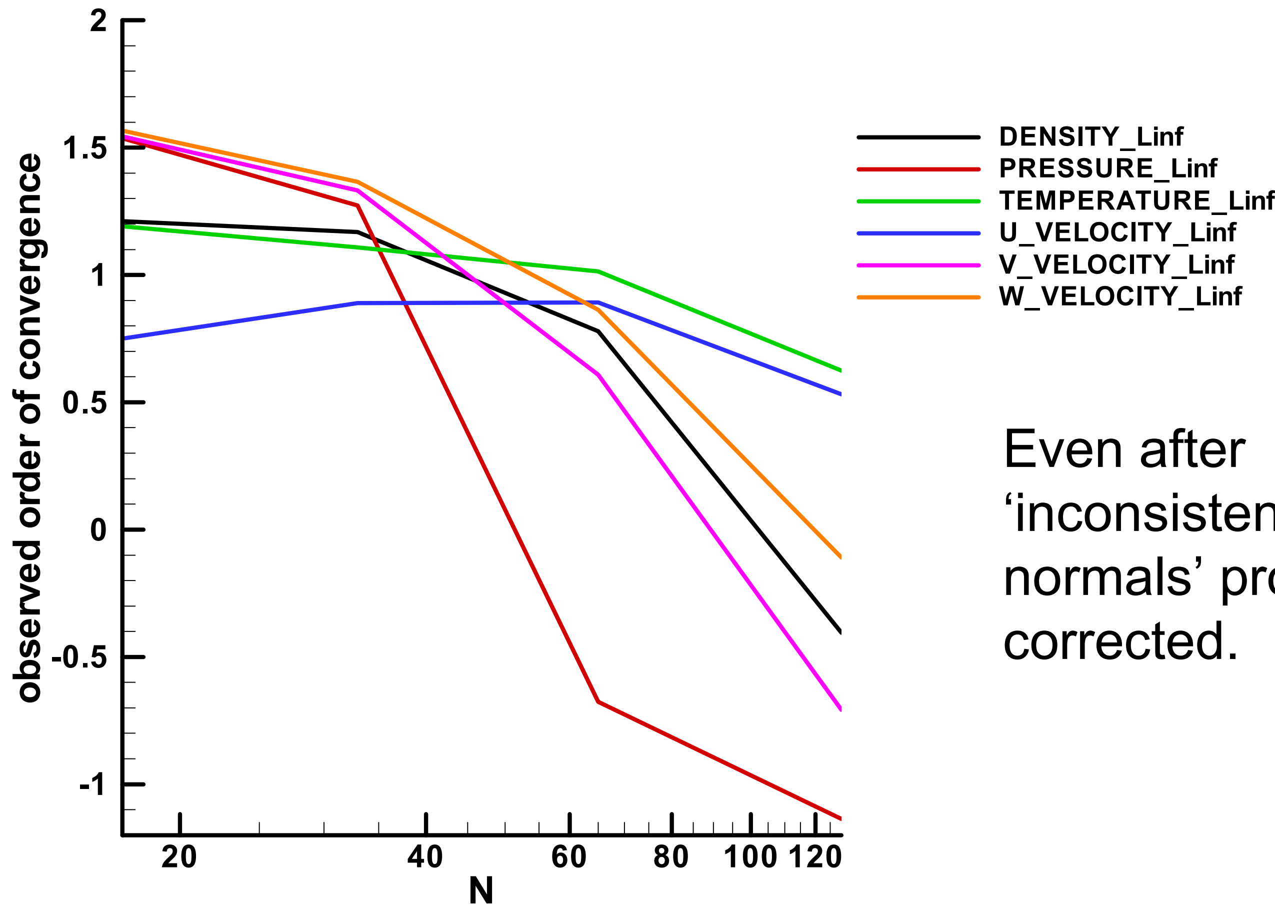
- The slip surface data lived on multiple processors on a parallel machine. The surface normals where the processor boundary intersected the slip surface were inconsistent between the processors because insufficient information provided across the processors. Code violated a known assumption of the parallelization algorithm.

Results on Second Try (after above problem corrected):

- Negative order-of-accuracy observed in all variables! (see next slide)

Slip Condition

Negative order of accuracy!



Even after 'inconsistent normals' problem corrected.

Discussion of Slip Results

- Negative order-of-accuracy in MMS results indicates non-convergence to solution.
- To date, no coding mistakes have been identified as the cause.
- Other non-MMS tests do not indicate non-convergence of measured quantities, although these tests are not as general as the MMS tests.
- Whether an unidentified coding mistake exists, or whether there is a problem with the MMS test itself is not known at this time. More work needed.

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Test 6

Test Setup:

- Solving Euler Equations,
- Mixed subsonic and supersonic outflow on G=0,
- Dirichlet elsewhere,
- Green-Gauss gradient reconstruction

Results: observed 2nd-order of accuracy in density, pressure, and velocity (see AIAA2004-2629)

Conclusions:

- The mixed subsonic & supersonic test of the outflow condition was observed to be second-order, extending the verification of the outflow condition to the full range of Mach numbers.
- Probably the first demonstration that MMS can be successfully applied to the testing of outflow boundary conditions on production CFD code.

Test 7

Test Setup:

- Solving Navier-Stokes,
- Dirichlet boundary conditions everywhere & on all variables,
- Green-Gauss gradient reconstruction

Results on First Try:

Observed zero-order accuracy on the coarsest meshes,

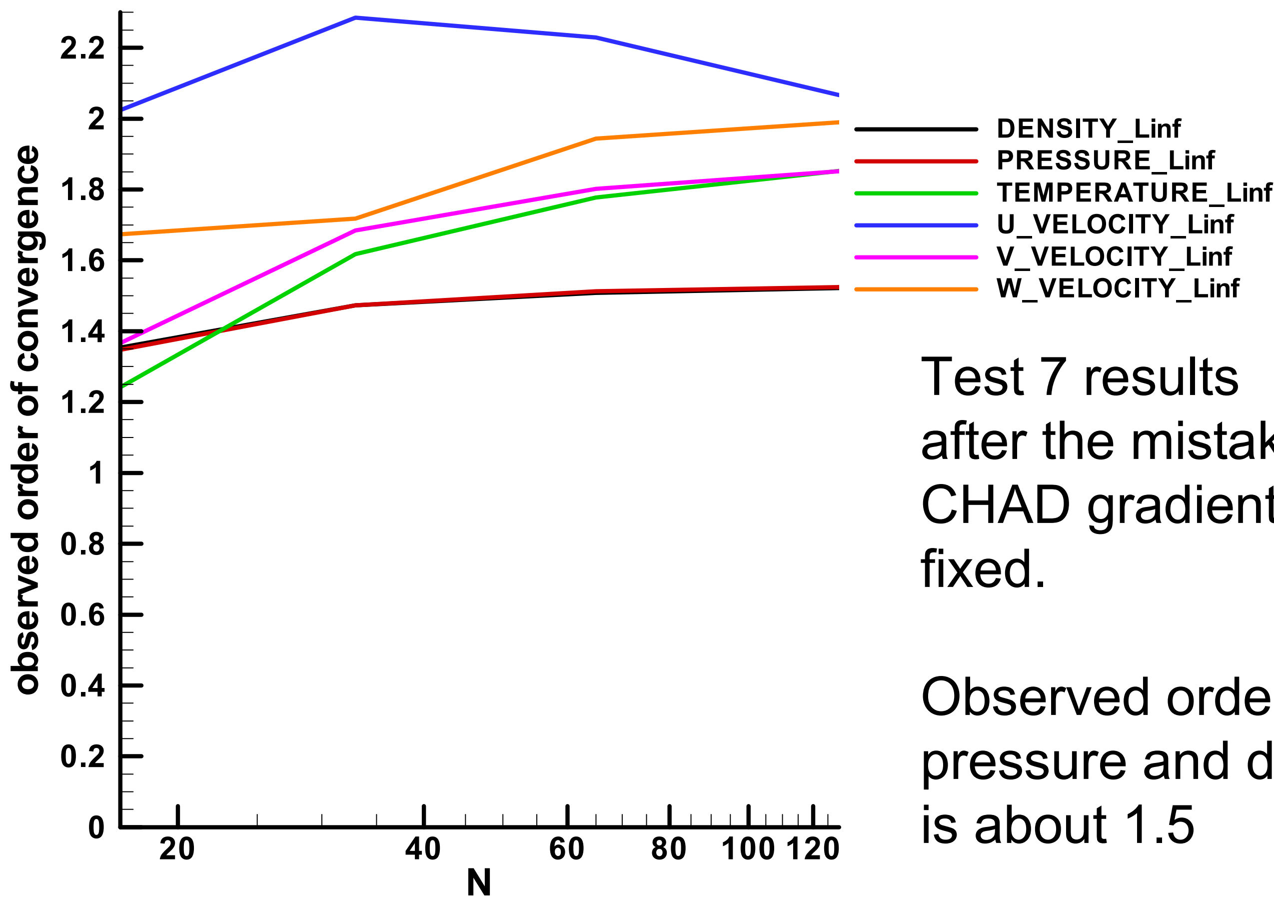
Test 7

Explanation of Zero-order behavior:

- It was observed that the error went to zero along edges which were aligned with one of the coordinate axes,
- Investigation revealed a coding mistake in the CHAD gradient correction,
- Mistake went undetected in prior MMS verification work (Roy, AIAA2002-3110) because aligned Cartesian meshes were used to reduce computational cost
- As a bonus, another unrelated mistake in an unused code option was found while looking for the CHAD mistake! (Incorrect calculation of thermal conductivity when viscous flux option selected). This mistake may have been found by later MMS testing.

Runs were repeated after the mistake was fixed (see next slide).

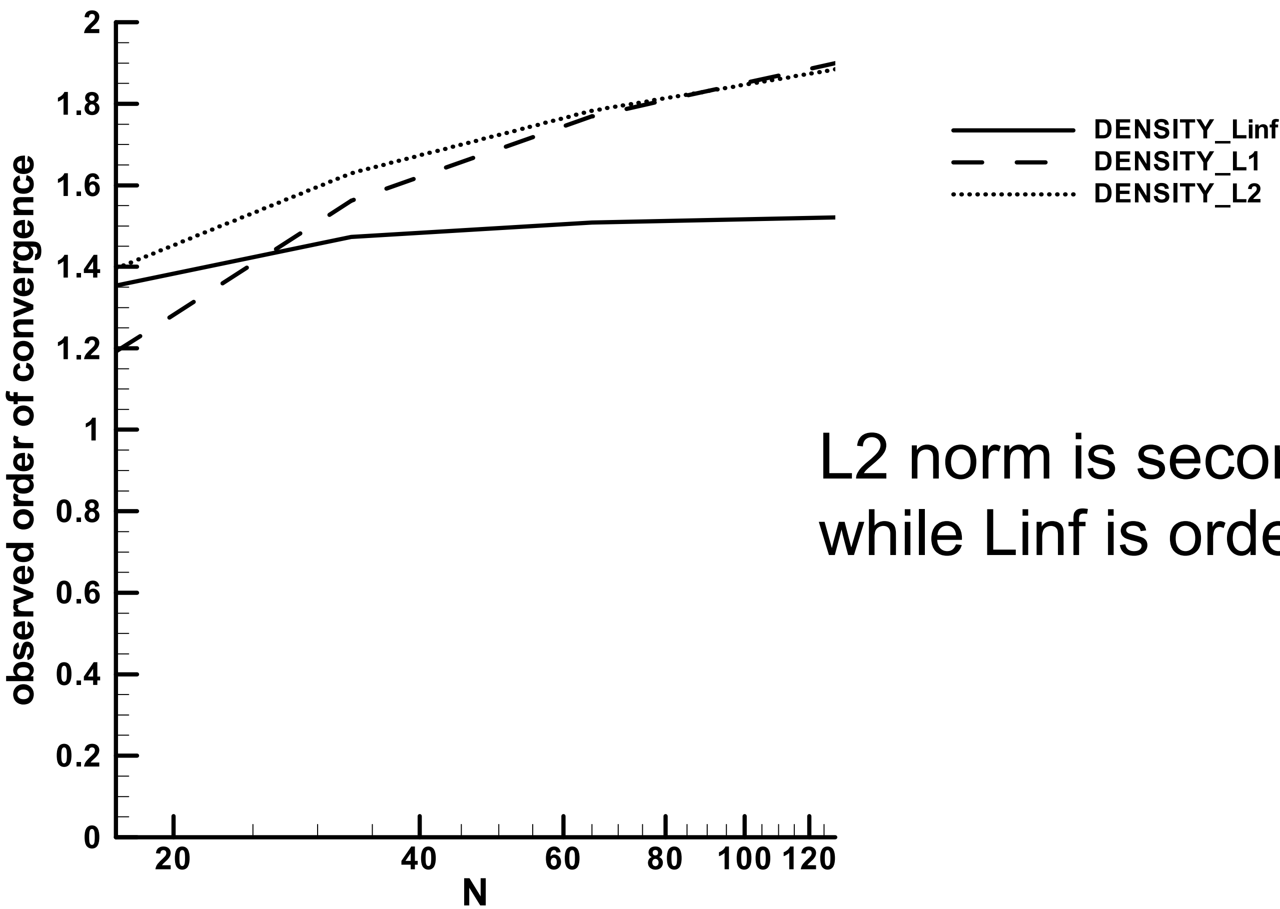
Navier-Stokes Results



Test 7 results after the mistake in CHAD gradient fixed.

Observed order of pressure and density is about 1.5

Observed Order of Density



L2 norm is second order while Linf is order 1.5

Explanation of Navier-Stokes Results

Explanation of Test 7, Second Try Results:

- The observed 1.5 order in density & pressure appears to be restricted to the F=0 boundary
- First Hypothesis: The slightly reduced order of convergence may be the result of using a compressible algorithm in the incompressible limit. Shot down by additional tests with higher Mach numbers
- Current hypothesis: CHAD correction is a tradeoff between accuracy and robustness, i.e., to minimize grid decoupling in viscous term one has to sacrifice second-order accuracy. This may explain the results on previous slide.

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Test 7

Interim Conclusions:

- Important coding mistakes will go undetected with insufficiently general tests. MMS provides a means of constructing these general tests.
- Ultimately, all coding mistakes are found by scrutinizing source code. The intensity of the scrutiny goes up dramatically when a coding mistake is suspected, and even more when the nature of the possible mistake is known. The bonus mistake was found because the particular routine was thought to contain the mistake when in fact it did not.

Test 8

Test Setup:

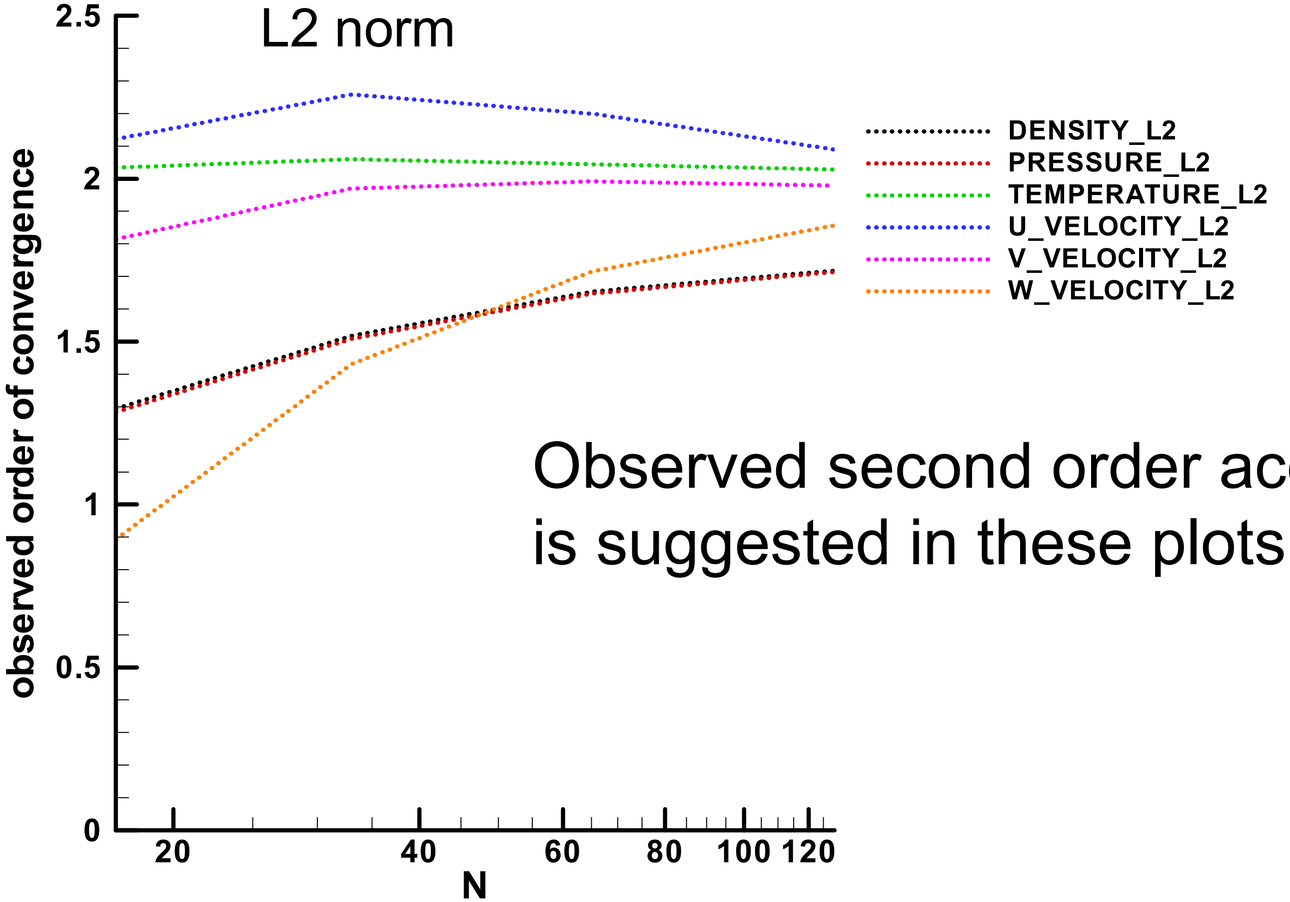
- Solving Navier-Stokes,
- No-slip, adiabatic,
- Dirichlet boundary conditions everywhere & on all variables,
- Green-Gauss gradient reconstruction

Results of First Try:

- Second order accuracy observed for temperature,
- First order accuracy observed for density and pressure, but only on the boundary,
- See next two slides.

Adiabatic No-Slip Condition

Error Calculation Performed over Entire Domain, L2 norm



Observed second order accuracy is suggested in these plots.

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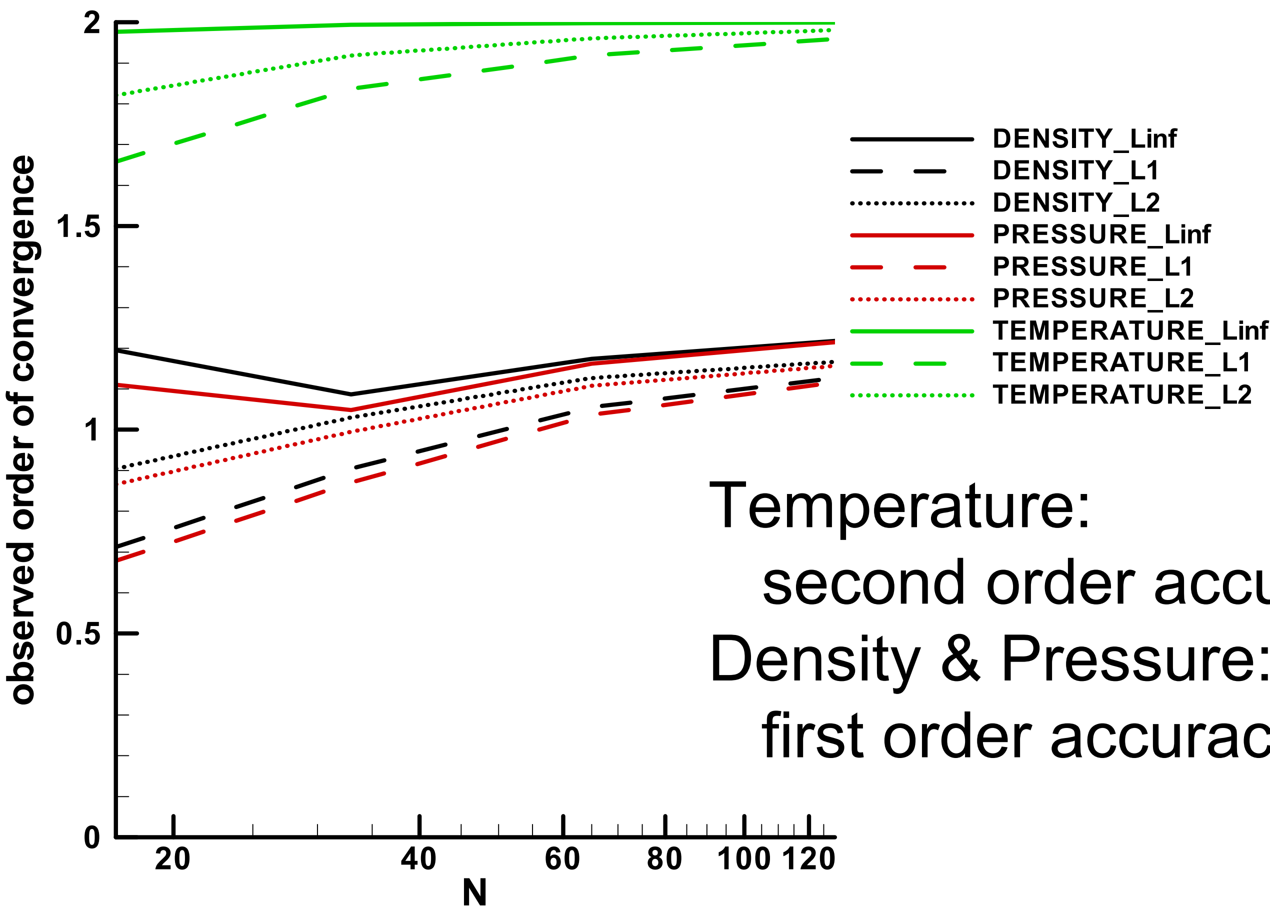
Adiabatic No-Slip Condition

Error Calculation Restricted to No-Slip Surface



Temperature:
second order accuracy

Density & Pressure:
first order accuracy

Boundary versus Interior Error

Explanation:

- For hyperbolic or parabolic equation sets, it is possible for error generated at a boundary to propagate out of the domain or remain on the boundary surface, rather than propagating into the interior.
- Whether this happens depends upon the variables in which the error is generated and the direction of characteristics at the surface.
- Because the boundary nodes compose a smaller fraction of the total as the mesh is refined, this situation results in order p convergence of the L_2 and L_1 norms, even when order $p - 1$ error is generated on the boundary.

Test 8

Conclusions:

- For non-elliptic systems, order-of-accuracy using L2 error norm may overlook lower order error confined to an outflow boundary
- No further investigation of this case is planned because first order accuracy is expected and explained on the boundary.

Test 9

Isothermal no-slip results in Test 9 look very similar to the adiabatic no slip results but still running on the 129x129x129 grid.

Conclusions

- A coding mistake in the CHAD gradient correction (to remove odd/even decoupling) was identified and corrected.
- An unresolved issue exists with the slip condition test, so further investigation is warranted.
- Order 1.5 in density and pressure was observed in a region of the Navier-Stokes test:
  - Latest hypothesis: order-of-accuracy of CHAD gradient correction is not always two
  - A future run will be performed to test this hypothesis.

Conclusions (2)

- All boundary conditions except the slip condition have been verified to their expected orders of accuracy.
- The coding mistake with the least squares gradient in prior work has been corrected and verified.
- Changes made to the manufactured solution have allowed better attainment of the asymptotic regime on the chosen sequence of meshes.
- Future work will focus on verifying the Reynolds-Averaged Navier-Stokes equations as well as dealing with unresolved issues such as slip.
- Verification of non-steady flow using MMS remains.

Lessons Learned

- Exact solutions can be manufactured to test slip, no-slip, and outflow boundary conditions,
- Demonstrated (for the very first time!) the feasibility of verifying a mixed subsonic/supersonic outflow boundary condition via MMS,
- Testing on non-orthogonal meshes revealed hidden coding mistake not found with Cartesian meshes,
- Both coding and algorithmic mistakes were uncovered,
- MMS usually cannot be applied blindly but takes understanding of the code, it's algorithms, and how to troubleshoot,
- Prior tests of Premo using MES did not test any boundary conditions. Even had they done so, coverage would not be as complete because simplifications of the PDE's would have been required.

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